

CLAIMS

What is claimed is:

1. Computer apparatus for determining state of physical properties of a chemical process:
 - 5 steady state modeling means for rigorously modeling a chemical process at steady state, the chemical process including physical properties, said steady state modeling means providing values for the physical properties at steady state based on a rigorous model of the chemical process; and
 - 10 an inferential model means coupled to receive the values of the physical properties at steady state from the steady state modeling means, the inferential model means for determining state of the physical properties over a period of time based on values of the physical properties at steady state.
2. Computer apparatus as claimed in claim 1 wherein the physical properties include melt index, density, tacticity, molecular weight distribution, xylene solubles, co-polymer composition and production weight.
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3. Computer apparatus as claimed in claim 2 wherein the steady state modeling means computes values of the physical properties in terms of molecular weight distribution, and
 - 20 the inferential model means correlates at least melt index and density with molecular weight distribution.
4. Computer apparatus as claimed in claim 2 wherein the steady state modeling means further calculates an instantaneous residence time of a reactor in the chemical process; and

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the inferential model means calculates cumulative values for the physical properties by mixing the values of the physical properties at steady state, including at least melt index and density, with previously calculated cumulative values of the physical properties over the residence time as last calculated by the steady state modeling means.

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5. Computer apparatus as claimed in claim 1 wherein the inferential model means utilizes a first order dynamics of mixing analysis with most recent values of the physical properties at steady state provided by the steady state modeling means, to calculate cumulative values of the physical properties.
- 10 6. Computer apparatus as claimed in claim 1 wherein the inferential model means further receives as input, off-line measured values of the physical properties and adjusts the determined state of the physical properties based on the received off-line measured values of the physical properties.
- 15 7. Computer apparatus as claimed in claim 1 wherein the inferential model means calculates and outputs values of parameters, of the chemical process, for maintaining the physical properties at a user specified state; and
the apparatus further comprises a process control subsystem coupled to receive the parameter values output from the inferential model means, such that the process control subsystem controls the chemical process according to the
20 parameter values.
8. Computer apparatus as claimed in claim 7 wherein the process control subsystem includes sensors measuring physical conditions of the chemical process; and
the inferential model means updates sensor measurements.

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9. A method for determining state of physical properties of a chemical process, comprising the computer implemented steps of:
- rigorously modeling a subject chemical process at steady state, including modeling physical properties of the chemical process at steady state, said modeling providing instantaneous physical property values for a given time, indicative of respective physical properties at steady state; and
- using the instantaneous physical property values, estimating state of the physical properties over a period of time using a first order dynamics of mixing analysis, such that estimates of the physical properties are dynamically calculated based on a rigorous steady state model.
10. A method as claimed in claim 9 wherein the physical properties include melt index, density, tacticity, molecular weight distribution, xylene solubles, co-polymer composition and production weight.
11. A method as claimed in claim 10 wherein the step of modeling includes computing values of the physical properties in terms of molecular weight distribution; and
- the step of estimating includes correlating at least melt index and density with molecular weight distribution.
12. A method as claimed in claim 10 wherein the step of modeling includes calculating an instantaneous residence time of a reactor in the subject chemical process; and
- the step of estimating includes calculating cumulative values for the physical properties by mixing the instantaneous physical property values with previously calculated cumulative values of the physical properties over the residence time as last calculated by the modeling step.

13. A method as claimed in claim 9 further comprising the step of receiving off-line measured values of the physical properties and adjusting the estimated state of the physical properties based on the received off-line measured values.
14. A method as claimed in claim 9 further comprising the step of calculating values
5 of parameters of the subject chemical process for maintaining the physical properties at a user specified state.
15. A method as claimed in claim 14 further comprising the step of updating sensor measurements of physical conditions of the subject chemical process.
16. Computer apparatus for process control, comprising:
10 a steady state modeler for modeling a subject process including physical properties at steady-state, the steady-state modeler providing a steady state model of the subject process;
an inferential sensing member coupled to the steady state modeler for determining state of physical properties over a period of time, such that a
15 dynamic model of the subject process is formed from the steady state model, the inferential sensing member further providing parameter values for maintaining physical properties at a user specified state in the subject process to effect control of the process; and
a network communication assembly coupled to the steady state modeler
20 and the inferential sensing member enabling online and user-interactive access to at least one of the steady state model, the dynamic model and parameter values, for enabling control of the subject process.
17. Computer apparatus as claimed in Claim 16 wherein the subject process is a
25 chemical process, or polymer process, or physical process carried out in a processing plant.

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18. Computer apparatus as claimed in Claim 17 wherein the parameter values are usable for defining state of equipment forming the processing plant.
19. Computer apparatus as claimed in Claim 16 wherein the steady state modeler computes instantaneous state of the physical properties of the subject process in terms of molecular weight distribution; and
- 5 the inferential sensing member includes an integrator for correlating certain physical properties with molecular weight distribution and updating sensor measurements of other physical properties, said integrator integrating changes in the certain physical properties based on the steady state modeler computed instantaneous states of the physical properties.
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20. Computer apparatus as claimed in Claim 19 wherein the certain physical properties include melt index, density, tacticity, molecular weight distribution, xylene solubles, co-polymer composition and production weight.

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